

## The electronic spectrum of silicon monotelluride radical

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**Abstract.** In the electronic spectrum of silicon monotelluride which has been produced in microwave discharges through sealed tubes, a large number of new bands belonging to the  $A^1\Pi-X^1\Sigma^+$  system (3100–3900 Å) and the  $E^1\Sigma^+-X^1\Sigma^+$  system (2800–3100 Å) of  $\text{Si}^{130}\text{Te}$  has been observed. The vibrational structure analyses of these band systems have resulted in the determination of improved vibrational constants in all the three electronic states involved in these transitions. An error in the previous determination of the vibrational constants of the  $E^1\Sigma^+$  state has been corrected. An upper limit for the dissociation energy of the silicon monotelluride has been determined to be  $40,000\text{ cm}^{-1}$ .

**Keywords.** Electronic spectrum; SiTe radical.

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### 1. Introduction

Barrow (1939) and Vago and Barrow (1946a, b) investigated the electronic spectrum of the silicon monotelluride (SiTe) in which they identified two band systems:  $A^1\Pi-X^1\Sigma^+$  (3100–3900 Å) and  $E^1\Sigma^+-X^1\Sigma^+$  (2800–3100 Å). Bosser and Lebreton (1983) carried out the rotational analysis of a few bands belonging to the  $A-X$  system. We have been investigating the electronic spectra of ten valence electron diatomic systems: SiO, SiS, SiSe and SiTe. We have recently undertaken the study of the emission spectrum of the SiTe radical under moderate as well as high resolutions. During these studies we have recorded the  $A-X$  and  $E-X$  bands of the isotopic radical  $\text{Si}^{130}\text{Te}$ . We have been able to identify a number of new bands belonging to these band systems. A close scrutiny of their vibrational structure revealed that the vibrational constants determined by Vago and Barrow (1946b)  $E^1\Sigma^+$  state are in error. The present investigation of the vibrational structure of these band systems has resulted in the determination of improved vibrational constants. These results are reported in this communication.

### 2. Experimental details

While Vago and Barrow (1946b) have obtained the absorption spectrum of SiTe by preparing the silicon monotelluride in situ by a chemical process, Bosser and Lebreton (1983) produced its emission spectrum in a Schuler type of hollow cathode discharge tube. These methods require gramme quantities of silicon and tellurium. Since the expensive enriched isotopes are available only in milligram quantities, neither

of these methods is suited for producing the electronic spectra of isotopic molecules ( $\text{Si}^{128}\text{Te}$  and  $\text{Si}^{130}\text{Te}$ ). We have, therefore, employed in the present studies the microwave excitation which requires only milligramme quantities of the substances. The electronic spectrum of  $\text{Si}^{130}\text{Te}$  is produced by running microwave discharge (2450 MHz, 100 W) through a sealed quartz tube containing milligramme quantities of silicon and tellurium isotope  $^{130}\text{Te}$  (99.9% enriched) along with neon gas at a pressure of about 2 Torr. The discharge tube is heated by a furnace which is in the form of a current-carrying wire wound around the discharge tube in order to generate sufficient vapour pressure of  $\text{SiTe}$ . This method of excitation produces strong and clean spectrum of the  $\text{SiTe}$  radical. The spectrum has been photographed in the first order of a 3.4 m Ebert grating spectrograph at a dispersion of  $5 \text{ \AA}/\text{mm}$ . The bandheads have been measured on Abbe comparator using iron lines as standards. The relative accuracy of the bandhead measurements is expected to be  $\pm 0.5 \text{ cm}^{-1}$  for sharp heads.

### 3. Results and discussion

#### 3.1 $A-X$ system

The  $A-X$  system lies in the 3100–3900  $\text{\AA}$  region. It is very strongly produced by the present method of excitation. The  $A-X$  bands are red degraded, most of them possessing sharp heads. In the present studies many new bands belonging to this system have been identified and their vibrational assignments made. All the bands belonging to the  $A-X$  system are presented in table 1. They have been fitted by a

**Table 1.** Bandheads of the  $A^1\Pi-X^1\Sigma^+$  system of  $\text{SiTe}$ .

Band $v'-v''$	Wavelength ( $\lambda$ ) $\text{\AA}$	Wavenumber ( $\text{cm}^{-1}$ )		$\Delta v =$ $\nu_{\text{obs}} - \nu_{\text{cal}}$
		RFB's data	Present data	
12-2	3181.05		31427.11	-2.23
8-0	3207.29		31169.98	-2.29
11-2	3211.52		31128.94	-2.79
9-1	3224.79		31000.81	-1.07
7-0	3239.62		30858.93	-2.19
10-2	3242.46		30831.89	1.16
8-1	3256.88		30695.39	1.27
6-0	3272.40		30549.80	3.21
9-2	3274.83		30527.15	0.80
7-1	3290.35	30384.7	30383.12	0.15
5-0	3307.11	30232.2	30229.15	0.47
6-1	3324.57	30071.0	30070.45	2.01
4-0	3343.19	29911.8	29902.98	-4.40
5-1	3360.29		29750.82	0.29
3-0	3379.42	29586.9	29582.33	-0.38
4-1	3396.75		29431.45	2.22
5-2	3414.81		29275.87	0.87
2-0	3417.18	29256.8	29254.67	0.03
6-3	3432.73		29122.98	2.98
3-1	3435.10		29102.89	-1.66

(Continued)

Table 1. (Continued)

Band $v'-v''$	Wavelength ( $\lambda$ ) Å	Wavenumber ( $\text{cm}^{-1}$ )		$\Delta\nu =$ $\nu_{\text{obs}} - \nu_{\text{cal}}$
		RFB's data	Present data	
4-2	3452.85	28955.5	28953.24	-0.46
1-0	3456.39	28925.3	28932.68	0.48
5-3	3470.87		28802.97	0.89
11-7	3471.59		28797.00	3.64
2-1	3473.95	28779.3	28777.44	0.95
9-6	3489.69		28647.67	-2.74
3-2	3492.03	28632.5	28628.44	-0.58
0-0	3496.87	28591.2	28588.87	0.50
10-7	3508.46		28494.35	1.99
4-3	3509.66		28484.66	3.87
1-1	3514.55	28446.9	28444.99	-0.06
5-4	3528.55		28332.16	0.37
6-5	3547.43		28181.35	-0.68
3-3	3550.70	28159.2	28155.45	-0.66
0-1	3556.41	28112.9	28110.20	-0.02
4-4	3569.02		28010.91	0.42
1-2	3574.24	27970.4	27970.01	0.49
2-3	3592.59	27829.2	27827.15	-0.90
6-6	3606.68		27718.43	1.46
3-4	3610.33		27690.43	4.61
0-2	3617.57	27637.2	27634.95	0.26
4-5	3630.15		27539.21	-3.61
2-4	3654.21	27358.4	27357.87	0.12
6-7	3668.83		27248.90	-5.64
3-5	3673.16		27216.76	-1.38
0-3	3680.64	27164.3	27161.45	-0.32
1-4	3699.39		27024.00	-2.31
5-7	3711.19		26937.86	1.24
2-5	3717.93		26889.02	-1.06
6-8	3730.74		26796.71	1.99
3-6	3736.66		26754.22	1.13
0-4	3745.57	26693.6	26690.63	-0.85
4-7	3756.11		26615.76	0.43
1-5	3763.87	26560.6	26560.86	2.23
3-7	3802.51		26290.95	0.30
0-5	3812.30		26223.41	-0.40
4-8	3821.92		26157.42	1.91
1-6	3831.38	26094.1	26092.81	-0.77
5-9	3842.04		26020.42	0.81
2-7	3850.87	25963.0	25960.79	-1.80
0-6	3881.10		25758.61	-0.14
1-7	3900.26	25629.7	25632.03	0.89
2-8	3920.08		25502.44	-0.33
3-9	3939.89		25374.21	0.57
0-7	3952.84		25297.48	1.16
1-8	3971.56		25171.92	0.59
2-9	3992.00		25043.02	-2.55

(Continued)

Table 1. (Continued)

Band $v'-v''$	Wavelength ( $\lambda$ ) $\text{\AA}$	Wavenumber ( $\text{cm}^{-1}$ )		$\Delta\nu =$ $\nu_{\text{obs}} - \nu_{\text{cal}}$
		RFB's data	Present data	
3-10	4012.40		24915.69	-3.37
4-11	4032.85		24789.38	-2.40
2-10	4065.97		24587.43	-3.57
3-11	4086.11		24465.23	-1.87
4-12	4107.33		24339.82	-2.62
2-11	4141.38		24139.76	0.72
4-13	4184.11		23893.23	-2.49

least squares program to the standard equation (Herzberg 1950) which yielded an improved set of vibrational constants for the  $X^1\Sigma^+$  and  $A^1\Pi$  states (table 3).

### 3.2 $E-X$ system

The  $E-X$  bands which were earlier studied in absorption (Vago and Barrow 1946b) have been recorded in emission in the present studies. The red degraded bands belonging to the  $E-X$  system of  $\text{Si}^{130}\text{Te}$  lie in the 2800–3100  $\text{\AA}$  region (Figure 1). A number of new bands belonging to this system have been observed in the present studies for which appropriate vibrational assignments have been made. As can be noticed from the figure most of the bands do not possess sharp heads. It has also been observed that, firstly, the intensity of the  $E-X$  bands compared to that of the  $A-X$  bands is much smaller, may be by a factor of 100. Secondly, the ratio of the intensity of the  $E-X$  system to that of the  $A-X$  system has been found to be considerably smaller in  $\text{SiTe}$  than the similar intensity ratio in  $\text{SiS}$  and  $\text{SiSe}$ . We have therefore faced considerable difficulty in photographing the  $E-X$  bands under high resolution. The vacuum wavenumbers of the bandheads together with their vibrational assignments are presented in table 2. They are fitted in a least squares program to the usual equation (Herzberg 1950) and the resulting constants are presented in table 3. The vibrational constant of  $242 \text{ cm}^{-1}$  obtained by Vago and Barrow of  $E^1\Sigma^+$  state is clearly in error. In fact the least squares fitting of their own data yielded  $234 \text{ cm}^{-1}$ . The anharmonicity terms obtained by them are unusually large. In analogy to the  $E-X$  bands of  $\text{SiS}$  and  $\text{SiSe}$ , (Lakshminarayana *et al* 1985; Lakshminarayana and Shetty 1988), we have not been able to find any  $E-X$  bands of  $\text{SiTe}$  that may be expected to occur in the visible region. We suppose that in  $\text{SiTe}$  the intensity of the expected visible bands is very low, in line with the relatively low intensity of the  $E-X$  bands in the ultraviolet region. Another problem was the persistent occurrence of  $\text{Te}_2$  bands in the 4000–6000  $\text{\AA}$  region in which the visible  $E-X$  bands are expected to occur.

### 3.3 Dissociation energy of $\text{SiTe}$

The dissociation energy calculated from the relation  $D_0 = \omega_0^2/4\omega_0x_0$  using the constants given in table 3 turns out to be  $46,000 \text{ cm}^{-1}$ . This value represents an upper limit to

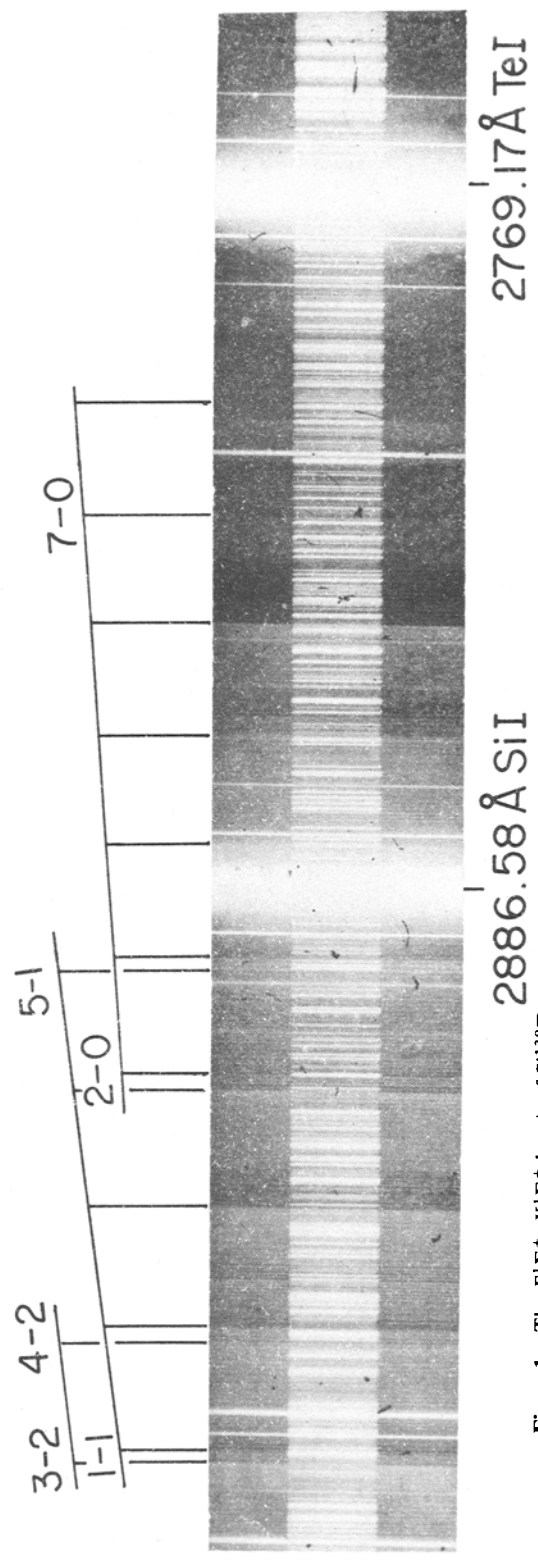
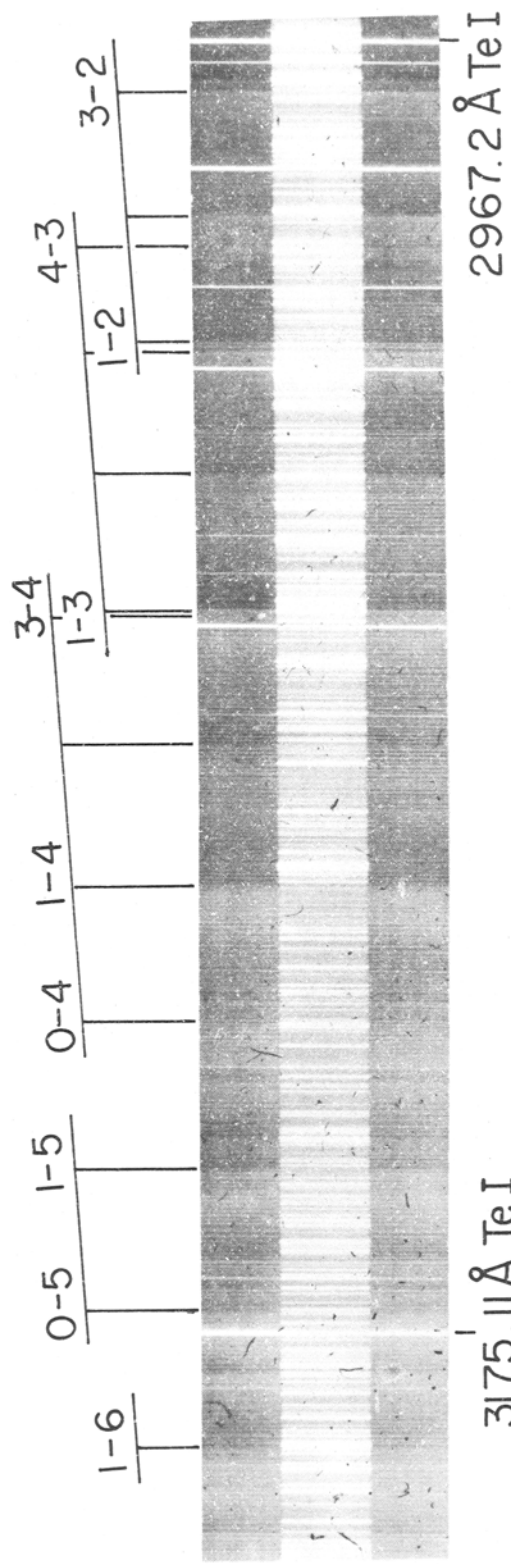


Figure 1. The  $E^1\Sigma^+ - X^1\Sigma^+$  bands of  $\text{Si}^{130}\text{Te}$ .

**Table 2.** Bandheads of the  $E^1\Sigma^+ - X^1\Sigma^+$  system of SiTe.

Band $v'-v''$	Wavelength ( $\lambda$ ) $\text{\AA}$	Wavenumber ( $\text{cm}^{-1}$ )		$\Delta v =$ $\nu_{\text{obs}} - \nu_{\text{cal}}$
		RFB's data	Present data	
8-0	2804.90		35641.39	10.19
7-0	2822.24		35422.37	1.99
6-0	2839.55	35210.1	35206.47	-0.69
5-0	2857.47	34991.9	34985.70	-5.87
4-0	2875.22	34772.4	34769.78	-3.83
3-0	2893.30	34552.7	34552.52	-0.74
5-1	2897.05	34513.9	34507.70	-6.08
2-0	2912.16	34330.2	34328.72	-1.81
4-1	2915.06	34295.7	34294.57	-1.24
3-1	2933.71	34074.7	34076.59	-1.12
2-1	2952.98	33854.5	33854.23	1.48
1-1	2972.94	33629.0	33626.95	-0.68
3-2	2975.12		33602.31	-2.05
2-2	2995.06	33379.4	33378.52	1.00
1-2	3015.62	33152.6	33150.99	-1.42
3-3	3017.24		33133.23	-5.62
0-2	3036.89	32918.5	32918.85	-6.07
2-3	3037.74		32909.68	4.79
1-3	3059.01	32680.1	32680.74	0.96
0-3	3080.59	32443.2	32451.89	-0.39
0-4	3125.72		31983.37	1.15
1-5	3149.17		31745.17	2.95
9-3	2905.23		34410.62	-3.37
9-4	2945.35		33941.86	-2.07
1-6	3196.18		31278.30	0.99

**Table 3.** Electronic and vibrational constants of SiTe ( $\text{cm}^{-1}$ ).

State	$T_e$	$\omega_e$	$\omega_e x_e$
$E^1\Sigma^+$	34000.31	229.86	1.190
$A^1\Pi$	28659.74	338.21	1.691
$X^1\Sigma^+$	0	480.77	1.309

the true value for  $D_0$ . A plot of  $\Delta G$  versus  $v$  has yielded a value of  $44300 \text{ cm}^{-1}$ . As this method involved a long extrapolation, the true value of  $D_0$  will be somewhat lower than this value. An examination of the plots of the dissociation energy and vibrational constants of SiO, SiS, SiSe and SiTe versus the atomic number leads to an estimated value of  $40,000 \text{ cm}^{-1}$  for the  $D_0$  of SiTe. This value may be compared with the corresponding value of  $37,000 \text{ cm}^{-1}$  obtained from thermochemical data which we feel is somewhat low (Huber and Herzberg) 1967).

## References

- Barrow R F 1939 *Proc. Phys. Soc.* **51** 267  
 Bosser G and Lebreton J 1983 *J. Phys.* **B16** 39

- Herzberg 1950 *Molecular Spectra and Molecular Structure* (New York: Van Nostrand) vol. 1  
Huber K P and Herzberg G 1979 *Molecular Spectra and Molecular Structure IV Constants of Diatomic Molecules* (New York: Van Nostrand Reinhold Company)  
Lakshminarayana G, Shetty B J and Sheila Gopal 1985 *J. Mol. Spectrosc.* **112** 1  
Lakshminarayana G and Shetty B J 1988 *J. Mol. Spectrosc.* **130** 155  
Vago E E and Barrow R F 1946a *Nature (London)* **157** 77  
Vago E E and Barrow R F 1946b *Proc. Phys. Soc.* **58** 538